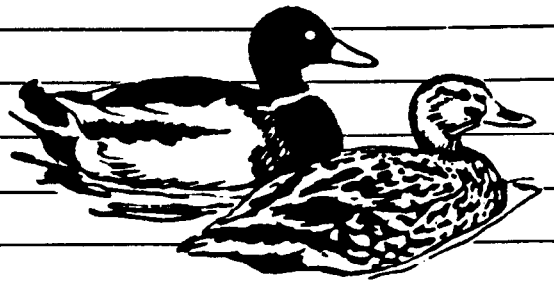
Research
Information bulletin
U.S. DEPARTMENT OF THE INTERIOR
NATIONAL BIOLOGICAL SURVEY



Number 91
1994

Integrating Software Technology and Laboratory Resources for Total Laboratory Quality

Integration of computer software and laboratory resources is a natural evolution. Laboratory software has revolutionized the way laboratories operate by providing an effective management tool for the analytical laboratory. We developed a software design and program to optimize laboratory information processing by providing facilities for automating the laboratory's data acquisition, processing, and archiving functions. The software design provides scientific and management information that can aid the planning and controlling of laboratory resources and related investigations, and it integrates with other laboratory scientific software through binary and ASCII (American Standard Code for Information Interchange) coding.

Laboratory measurement data are often the basis for critical decisions on integral matters, ranging from the health of individuals to the protection of the environment. The data used for such purposes must be reliable. Reliability is achieved through quality assurance. Quality assurance is maintained through the integration of software technology and laboratory resources by providing the dynamic abilities to work with multiple secured data bases on a single computer network shared by all laboratory divisions, to enforce standard operating procedures, to archive database information routinely, to assign worklists and scheduling, and to secure laboratory software and data.

Data Bases and Processing

The simplicity of the database system is achieved by storing data in an easy-to-visualize and familiar form—ASCII. A data base is developed from laboratory data (e.g., text, numerical, graphics) that traditionally would be stored and processed by using several combinations of commercial software; however, this system merges the data into multiple ASCII and binary files. The file is identified by a particular data type and is given a name, such as STDPROCE.TXT. Data

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bases developed in ASCII and binary format can use all data types and may contain text, numerical data, or graphics. The ASCII and binary files are the basic unit for all laboratory information maintained as digital code in the software. This exclusive data format clarifies database design and facilitates communication between laboratory resources and commercial software used for other tasks.

Resource managers and research scientists require state-of-the-art instrumentation, equipment, and physical laboratory facilities to develop and operate an overall program for ecosystem analysis and environmental management. We are integrating software technologies with laboratory resources through continued research and development of laboratory information management software technologies and tools. The laboratory offers a variety of resources, including atomic absorption, atomic fluorescence, and flame-emission spectrometry; molecular luminescence, absorption, and raman spectrometry; light scattering and refractometry–chiroptical methods; energetic particle and X-ray methods—mass and X-ray fluorescence spectrometry; gas and liquid gas chromatography; and potentiometric and hydrodynamic methods for sample analysis.

Scientific Implications

The user interface for the system allows the user to communicate with hundreds of laboratory data bases through menus and forms presented in a windows style. This manner of presentation is easy to understand, decreases the probability for user error in data processing and acquisition, and provides a means for supporting a credible laboratory quality assurance program.

In the laboratory, researchers and resource managers will use this new technology as an analytical support and information tool. The software design and program will provide compliance with sample and data validation and with Good Laboratory Practice Standards. The software architecture will provide for laboratory standard methods referencing and implementation, material safety and use data, instrument operating procedures, employee emergency contact information, worklists and scheduling, and specific instrument and equipment design features and capabilities.

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